# IUPAC Task Group on Atmospheric Chemical Kinetic Data Evaluation - Data Sheet HOx_VOC91



This datasheet last evaluated: June 2014; last change in preferred values: June 2014.

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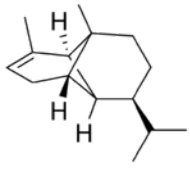
**OH +**  **(α-copaene) → products**

## Rate coefficient data

| $k$/cm$^3$ molecule$^{-1}$ s$^{-1}$ | Temp./K | Reference | Technique/Comments |
|---|---|---|---|
| *Relative Rate Coefficients* | | | |
| $(9.0 \pm 1.9) \times 10^{-11}$ | 296±2 | Shu and Atkinson, 1995 | RR (a) |

α-Copaene is (1R,2S,6S,7S,8S)-8-isopropyl-1,3-dimethyltricyclo[4.4.0.0$^{2,7}$]dec-3-ene

## Comments

(a) 6400 L Teflon chamber at 987 mbar (740 Torr) of air. OH radical was generated by the photolysis of $CH_3ONO$ at wavelengths > 300 nm. α-Copaene and 2,3-dimethyl-2-butene (reference reactant) were monitored by GC-FID. The rate constant ratio, $k$(OH + α-copaene) / $k$(OH + 2,3-dimethyl-2-butene) = 0.817 ± 0.044 is placed on an absolute basis using $k$(OH + 2,3-dimethyl-2-butene) = $1.1 \times 10^{-10}$ cm$^3$ molecule$^{-1}$ s$^{-1}$ at 298 K (Atkinson and Arey, 2003).

## Preferred Values

| Parameter | Value | T/K |
|---|---|---|
| $k$ /cm$^3$ molecule$^{-1}$ s$^{-1}$ | $6.7 \times 10^{-11}$ | 298 |
| *Reliability* | | |
| $\Delta \log k$ | 0.10 | 298 |

*Comments on Preferred Values*

The preferred value of the rate coefficient at 298 K is based on the relative rate coefficient determination of Shu and Atkinson (1995). The reaction is expected to proceed predominantly by addition to the >C=C< double bond.

## References

Atkinson, R., and Arey, J.: Chem. Rev., 103, 4605-4638, 2003.
Shu, Y., and Atkinson, R.: J. Geophys. Res., 100, 7275-7281, 1995.